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Abstract
The compilation of the material in this report was undertaken to provide a convenient reference source for intermetallic compounds. An adequate bibliography is required for most efficient use. It is in this sense and because of the addition of more compounds that the compilation is considered an extension of the compilation in Smithell's "Metals Reference Book."

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I. COMPOUNDS OF LITHIUM, SODIUM, POTASSIUM, AND RUBIDIUM.

by

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G. R. Kilp and J. F. Smith

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TABLE OF CONTENTS

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INTRODUCTION

The compilation of the material in this report was undertaken to provide a convenient reference source for intermetallic compounds. An adequate bibliography is required for most efficient use. It is in this sense and because of the addition of more compounds that the compilation is considered an extension of the compilation in Smithell's "Metals Reference Book."

Undoubtedly there are some compounds listed in the compilation which either do not exist or have been assigned the wrong formulae. It seems obvious, for instance, that not all of the reported sodium-mercury compounds should exist. For purposes of evaluation, the experimental basis for the report of a compound is included under "Remarks" after the compound.

The material is separated into three sections. The first part consists of a tabulation and includes the crystal class, lattice parameters, and Strukturbericht structure symbol or space group symmetry if the data have been reported. The second part of the compilation is the list of references, and the third part is a summary of structure details. The structure details include the space group symmetry, the number of atoms per unit cell, the atomic coordinates, and a list of compounds assigned to the structure.

PART I: TABULATION OF COMPOUNDS

COMPOUNDS	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
LiAg	cubic	a=3.17	B2	X-ray powder data, numerical intensities, thermal analysis, metallography.	1,2,3,4
Li_3Ag	cubic	a=9.96	$D8_{1-3}$	X-ray powder data, qualitative intensities, numerical intensities; formulae Li_9Ag_4, $Li_{10}Ag_3$, and $Li_{12}Ag$ also reported and are probably indicative of a region of solid solubility.	1,2, 5
$\sim Li_{20}Mg_{80}$				Some evidence for superlattice, possibly Fe_3Al type below ~420°C; superlattice formulae reported also as Li_3Mg_5, cubic with a=9.7, and as Li_2Mg_5, cubic with a=3.513; still in debate.	91,92, 6,7
$LiCa_2$				Thermal analysis and hardness data.	8
Li_2Ca	hexagonal	a=6.261 c=10.25	C14	X-ray powder data, numerical intensities.	9
$LiZn_9$	hexagonal	a=2.788 c=4.394	A3	Numerical intensities, x-ray powder data.	9,10
$LiZn_4$				X-ray powder data.	6
Li_7Zn_{18}	hexagonal	a=4.371 c=2.515	$[D^4_{6h}$-- $P6_3/mmc]$	X-ray powder data, numerical intensities, thermal analysis, electrical resistance; formulae Li_3Zn_7, $Li_{0.8}Zn_2$, and $LiZn_2$ also reported with same lattice parameters.	3,10,11

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Li_2Zn_3	cubic	a=4.27		Thermal analysis, electric resistance, and x-ray powder data.	3,6,11
LiZn	cubic	a=6.222	B32	X-ray powder data, numerical intensities.	3,4
$LiCd_3$	hexagonal	a=3.089 c=4.899	A3	X-ray powder data, numerical intensities, thermal analysis, conductivity and dilatometric data.	12,13
$LiCd_3$	cubic	a=8.62	complicated cubic	X-ray powder data, thermal analysis.	3,14
$LiCd_2$				Phase diagram.	15
LiCd	cubic	a=6.701	B32	X-ray powder data, numerical intensities.	4,12
LiCd	cubic	a=3.33	B2	X-ray powder data, numerical intensities, thermal data.	3,16,14
Li_3Cd	cubic	a=4.259	A1	X-ray powder data, numerical intensities, thermal analysis.	3,12,16
$LiHg_5$				Phase diagram--doubtful.	17
$LiHg_3$	hexagonal	a=6.253 c=4.804	DO_{19}	X-ray powder data, numerical intensities, thermal analysis.	3,18,19
$LiHg_2$				"	18,19
LiHg	cubic	a=3.24	B2	X-ray powder data, numerical intensities; parameter values reported as high as 3.294.	3,4,18,19
Li_2Hg				X-ray powder data, thermal analysis.	18,19

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Li_3Hg	cubic	a=6.561	DO_3	X-ray powder data, numerical intensities, thermal analysis.	18,19
Li_6Hg				Thermal analysis.	19
LiAl	cubic	a=6.372	B32	X-ray powder data, qualitative intensities, thermal analysis, temperature-resistance and micrographic data.	20,21 22,23, 24
Li_2Al				Thermal analysis, temperature-resistance and micrographic data.	23,24
LiGa	cubic	a=6.208	B32	X-ray powder data, numerical intensities.	3,4
LiIn	cubic	a=6.800	B32	X-ray powder data, numerical intensities, thermal analysis.	3,4,19
Li_2Tl_3				Thermal analysis and temperature-resistance data.	25
LiTl	cubic	a=3.431	B2	Thermal analysis, x-ray powder, numerical intensity and temperature-resistance data.	3,4,25
Li_2Tl				Thermal analysis and temperature-resistance data.	25
Li_5Tl_2				"	25
Li_3Tl				"	25
Li_4Tl				"	25
Li_2Si				X-ray powder data; no intensities given.	26
Li_4Si				"	26

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
$LiSn_4$				Thermal analysis.	27
Li_2Sn_5				Thermal analysis and temperature-resistance data.	15,28
$LiSn_2$				"	27,28
LiSn				Thermal analysis, temperature-resistance data, x-ray powder data; no intensities given.	27,28,4
Li_3Sn_2				Thermal analysis.	15,27
Li_2Sn				Thermal analysis and temperature-resistance data.	27,28
Li_5Sn_2				"	27,28
Li_7Sn_2				"	27,28
Li_4Sn				"	27,28
LiPb	cubic	a=3.529	B2	Thermal analysis, temperature-resistance and x-ray powder data.	4,29,30
Li_5Pb_2				Thermal analysis and temperature-resistance data.	30
$Li_{10}Pb_3$	cubic	a=10.010	$D8_3$	X-ray powder data, numerical intensities.	31
Li_3Pb	hexagonal	a=4.27 c=7.59	DO_{18}	Thermal analysis and temperature-resistance data.	30
Li_7Pb_2				"	30
Li_4Pb				"	30
Li_3N	hexagonal	a=3.665 c=3.890		X-ray powder data, numerical intensities.	32
Li_3N	cubic	a=5.51		X-ray powder data, qualitative intensities.	33

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Li_3P	hexagonal	a=4.273 c=7.594	DO_{18}	X-ray powder data, numerical intensities.	34
Li_3As	hexagonal	a=4.396 c=7.826	DO_{18}	"	34
α-Li_3Sb	hexagonal	a=4.710 c=8.326	DO_{18}	"	34
β-Li_3Sb	cubic	a=6.572	DO_3	"	34
LiBi	tetragonal	a=3.368 c=4.256	L1O	X-ray powder data, numerical intensities, thermal analysis and electrical resistances.	3,4,35
Li_3Bi	cubic	a=6.722	DO_3	Thermal analysis and electrical resistances.	3,35,36
Li_2S	cubic	a=5.720	C1	X-ray powder data, numerical intensities.	3,37
Li_2Se	cubic	a=6.017	C1	"	37
Li_2Te	cubic	a=6.517	C1	"	37
Na_2K	hexagonal	a=7.50±2 c=12.29	C14	X-ray powder data, Debye-Scherrer.	38
Na_2Cs				Thermal analysis.	39,50
NaAu				Existence questionable.	51

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
$NaAu_2$	cubic	a=7.7872 ± .0023	C15	X-ray powder data.	40,41, 59
Na_2Au	tetragonal	a=7.402 c=5.511	C16	Rotation, Weissenberg, and x-ray powder data.	41
$NaZn_{13}$	cubic	a=12.2836 ±0.0003	$D2_3$	X-ray powder data, comparison of F_o and F_c; F_o obtained by multiple film technique.	61,40
$NaCd_2$	cubic			X-ray powder data, thermal, micrographic, and electrical investigations.	42,53
$NaCd_5$				Thermal, micrographic, and electrical investigations.	53
$NaCd_6$				"	53
NaHg	orthorhombic	a=7.19 b=10.79 c=5.21	$[D_{2h}^{17}$-- Cmcm]	Weissenberg and precession x-ray data, visual estimation of intensities, least squares refinement of data; $R = \frac{\Sigma \lvert F_o - F_c \rvert}{\Sigma \lvert F_o \rvert} = 20.3\%$.	62
$NaHg_2$	hexagonal	a=5.0290 ±.0005 c=3.2304 ±.0016	C32	X-ray powder data.	62
$NaHg_4$	hexagonal	a=61.5 c=9.7		~230 $NaHg_4$ per cell; Weissenberg data.	62
$NaHg_5$				Thermal preparation (grown from melt); existence doubtful.	64
$NaHg_6$				"	64
$NaHg_7$				"	64

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
$NaHg_8$				Thermal preparation(grown from melt); existence doubtful.	64
$NaHg_9$				"	64
$NaHg_{10}$				"	64
$NaHg_{12}$				"	64
$NaHg_{14}$				"	64
Na_3Hg				Thermal analysis.	46
Na_3Hg_2	tetragonal	a=8.52 c=7.80	$/D_{4h}^{14}$-- $P4_2/mnm/$	Weissenberg and precession x-ray data, visual estimation of intensities refined by electron density maps, least squares refinement of data.	62
Na_5Hg_2	rhombohedral	a=18.52 α=29°23'		Precession x-ray data.	62
Na_7Hg_8				Thermal analysis.	46
NaIn	cubic	a=7.312	B32	X-ray powder data.	43,59
NaTl	cubic	a=7.473	B32	"	44,59
$NaTl_2$				Thermal analysis and temperature-resistance data.	54
Na_2Tl				"	54
Na_4Tl				Thermal analysis; existence questionable.	47
Na_6Tl				Thermal analysis and temperature-resistance data.	54,47
NaSi				Questionable; reported as formed by heating excess Na with Si in inert atmosphere, distilling off excess Na.	55

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
$NaSi_2$	tetragonal	a=4.98 c=16.7		X-ray powder data; possibility of different cell.	60
NaGe				Reported as formed by method used above for NaSi.	55
NaSn				Phase diagram.	66
$NaSn_2$				"	66
$NaSn_3$				"	66
$NaSn_4$				"	66
$NaSn_6$				"	66
Na_2Sn				"	66
Na_3Sn				"	66
Na_4Sn				"	66
Na_4Sn_3				"	66
Na_4Sn_9				Reported on basis of formation of precipitate, and discontinuity in potentiometric titration curve when Na was titrated with SnI_2 in aqueous NH_3.	67
$Na_{15}Sn_4$	orthorhombic	a=9.82 b=22.82 c=5.59	$\sim D8_6$	Powder, rotation, and Weissenberg x-ray data.	45
NaPb	tetragonal	a=10.580 ±0.005 c=17.746 ±0.015	$[D_{4h}^{20}$ -- I4/acd]	Crude single crystal data plus x-ray powder data; least squares refinement of Pb positions; (F_o-F_c) refinement of Na positions; powder intensities gotten by comparison with calibrated film. H^o_{298}= -11.6 kcal/mol.	63,59
Na_2Pb				Phase diagram.	17

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Na_2Pb_5		a=4.88	L12	Conflicting x-ray evidence about compound's existence.	17,65
Na_4Pb				Phase diagram.	17
Na_4Pb_7	cubic	a=4.873		Reported on basis of precipitation during potentiometric titration, and discontinuity in potentiometric titration curve.	67,3
Na_4Pb_9				"	67
Na_5Pb_2				Phase diagram.	17
$Na_{15}Pb_4$	cubic	a=13.31	$D8_6$	Powder, rotation, and Weissenberg x-ray data; visual estimation of intensities.	45,3
$Na_{31}Pb_8$		a=13.27		78 atoms per cell.	69,94
Na_3P	hexagonal	a=4.99 c=8.81	DO_{18}		34
Na_3As	hexagonal	a=5.089 c=8.99	DO_{18}	X-ray powder data	34,59 67
Na_3As_3				Reported on basis of precipitation during potentiometric titration, and discontinuity in potentiometric titration curve	67
Na_3As_5				"	67
Na_3As_7				"	67
NaSb				Analog of NaBi	44,67
Na_3Sb	hexagonal	a=5.367 c=9.515	DO_{18}		34

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
NaBi	tetragonal	a=3.47 c=4.81	L1O	Superlattice; x-ray powder data.	44,59,3
Na_3Bi	hexagonal	a=5.459 c=9.674	DO_{18}	X-ray powder data.	34,59
Na_3Bi_5				Reported on basis of precipitation during potentiometric titration, and discontinuity in potentiometric titration curve.	67
Na_2O	f.c.cubic	a=5.56	C1	X-ray powder data, visual estimation of intensities.	37,49
Na_2S	f.c.cubic	a=6.526	C1	X-ray powder data.	37,59,3
Na_2S_2				Reported on basis of precipitation during potentiometric titration, and discontinuity in potentiometric titration curve.	67
Na_2S_3				"	67
Na_2S_4				"	67
Na_2S_5				"	67
Na_2S_6				"	67
Na_2S_7				"	67
Na_2Se	f.c.cubic	a=6.81	C1	"	37,67,3
Na_2Se_2				"	67
Na_2Se_3				"	67
Na_2Se_4				"	67
Na_2Se_5				"	67
Na_2Se_6				"	67

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
NaTe				Reported on basis of precipitation during titration, and discontinuity in potentiometric titration curve; thermal analysis.	57,67
$NaTe_3$				Phase diagram; thermal analysis.	57
Na_2Te	f.c.cubic	a=7.32	C1	Thermal analysis.	57,37,3
Na_2Te_3				Reported on basis of precipitation during titration, and discontinuity in potentiometric titration curve.	67
Na_2Te_4				"	67
Na_4Th				Phase diagram; thermal analysis.	56
No K-Li compounds				Complete solid insolubility.	39
No K-Rb compounds				Complete solid solubility.	39
KCs				Very doubtful thermal analysis; later work (39) disputes evidence of CsK compound.	50,39
KAu_2 KAu_4				Both Au_2K and Au_4K were postulated on grounds of their x-ray powder spectra, which were distinctly different from both pure K and Au. No structures or parameters were determined from the x-ray patterns.	70

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
KAu				Determined by vacuum fusion--doubtful.	51
No K-Mg compounds				Complete solid immiscibility.	82
KZn_{13}	cubic	a=12.38	$D2_3$	X-ray powder data.	71,72
KCd_{13}	cubic	a=13.81	$D2_3$	"	71,72
KCd_7				Thermal analysis.	82
K_2Hg				Viscosity measurements in liquid amalgam indicated solid stable compound K_2Hg.	73
KHg_{12}				Determined $\Delta H_{form.}$, ΔF, and $\Delta H_{soln.}$ from emf.cells.	81
KHg	tri-clinic	a=6.62 b=6.91 c=6.94 α=106°, β=102°19', γ=92°48'	C_i^1--P$\bar{1}$	Precession x-ray data, single crystal; Patterson and electron density refinements.	80,93
KHg_2				Thermal analysis.	52
KHg_3				"	52
KHg_4				"	52
$KHg_{8 \text{ or } 9}$				"	52
KHg_{11}	cubic	a=9.65	O_h^1--Pm3m	(Same structure as $BaHg_{11}$.)	80,68
No K-Al compounds				Complete solid immiscibility.	82
K_2Tl				Thermal analysis, doubtful.	58

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
KTl				Thermal analysis; structure of KTl not isomorphous with NaTl, as determined by Debye-Scherrer method.	4,58
KSi_8				X-ray powder data and thermal analyses indicated existence of these compounds.	55
KSi				"	55
KGe				"	55
KGe_4				"	55
K_2Sn				Thermal analysis and phase diagram; (work done in 1907).	69
KSn				"	69
KSn_2				"	69
KSn_4				"	69
K_2Pb				"	76
KPb				"	76
KPb_2				Thermal analysis, phase diagram; compound checked with hardness tests and electrical resistivity by (83).	76,83
KPb_4				"	76,83
K_4Pb_9				Potentiometric titration of K with PbI_2 in liquid NH_3 gives sharp break at composition K_4Pb_9.	67

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
K_3As	hexagonal	a=5.793 c=10.242	DO_{18}	X-ray powder, Debye-Scherrer data.	34
K_3Sb	hexagonal	a=6.037 c=10.717	DO_{18}	"	34,74
KSb				Thermal analysis.	48
K_3Bi	hexagonal	a=6.180 c=10.955	DO_{18}	Debye-Scherrer x-ray powder data.	34,84
K_9Bi_7				Thermal analysis.	84
K_3Bi_2				"	84
KBi_2	cubic	a=9.52	C15	Debye-Scherrer x-ray powder data.	75,84
K_2Se	cubic	a=7.691	C1	Debye-Scherrer x-ray powder data.	37,77
K_2Se_2				Phase diagram constructed from thermal analysis; compounds determined by Debye-Scherrer x-ray powder method, but structures not determined.	77
K_2Se_3				"	77
K_2Se_4				"	77
K_2Se_5				"	77
K_2Te	cubic	a=8.168	C1	Debye-Scherrer x-ray powder data.	37,77
K_2Te_2				Phase diagram by thermal analysis and Debye-Scherrer x-ray powder data for compound determination, but structures not determined.	77

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
K_2Te_3				Phase diagram by thermal analysis and Debye-Scherrer x-ray powder data for compound determination, but structures not determined.	77
K_2Te_4				"	77
KRe				Paramagnetic properties of alloy of composition ReK indicates probable compound formation by Re with K.	78
No K-Fe compounds				Solid and liquid immiscibility.	79
$RbAu_2$ RbAu				Both gold compounds made by vapor diffusion; no structure details.	85
$RbCd_{13}$	cubic	a=13.88	$D2_3$	X-ray powder data.	71
$RbHg_9$				Compounds postulated by magnetic susceptability measurements and thermal analysis.	86,90
$RbHg_6$				"	86,90
Rb_2Hg_9				"	86,90
Rb_5Hg_{18}				"	86,90
Rb_2Hg_7				"	86,90
$RbHg_2$				"	86,90

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Rb_3Hg_4				Compounds postulated by magnetic susceptability measurements and thermal analysis.	86,90
Rb_7Hg_8				"	86,90
$RbHg_{11}$	cubic			Similar to KHg_{11}; no parameters determined.	87
$RbHg_{12}$	cubic	a=10.71			87
RbC_8	hexagonal	a=4.95 c=22.78		Method of preparation not given.	88
RbC_{16}	hexagonal	a=4.95 c=17.99		"	88
RbSi $RbSi_8$ RbGe $RbGe_4$				X-ray patterns of RbSi, $RbSi_8$, RbGe, and $RbGe_4$ were taken, but only shown, not worked out; samples prepared by direct union and subsequent volatilization of one component.	55
Rb_3Sb	hexagonal	a=6.29 c=11.23	$[D_{3h}^4$-- C6/mmc]	X-ray powder data; sample prepared by addition of alkaline metal vapor to solid Sb.	89

PART II: REFERENCES

1. Pastorello, S., Gazz. chim. ital. 60, 493 (1930).
2. Freeth and Raynor, J. Inst. Metals 82, 569 (1954).
3. Taylor, A., "X-Ray Metallography," pp. 373-375 (John Wiley & Sons Inc., New York, 1952).
4. Zintl and Brauer, Z. physik. Chem. B20, 245-252 (1933).
5. Perlitz, H., Z. Krist. 86, 155 (1933).
6. Baroni, A., Congr. intern. quím pura y apl.--Frab. IX 2, 75 (1934).
7. Grube, V. Zeppelin, and Bumm, Z. Elektrochem. 40, 160 (1934).
8. Zamatorin, M., Metallurgist 1, 96 (1938).
9. Hellner and Laves, Z. Krist. 105, 134 (1943).
10. Zintl and Schneider, Z. Elektrochem. 41, 764 (1935).
11. Grube and Vosskühler, Z. anorg. Chem. 215, 211 (1933).
12. Zintl and Schneider, Z. Elektrochem. 41, 294 (1935).
13. Grube, Vosskühler, and Vogt, Z. Elektrochem. 38, 869 (1932).
14. Baroni, A., Atti accad. naz. Lincei, Rend. 6 18, 41 (1933).
15. Masing and Tammann, Z. anorg. Chem. 67, 183 (1910).
16. Baroni, A., Z. Elektrochem. 40, 565 (1934).
17. Hansen, M., "Aufbau der Zweistofflegierungen," p. 919 (Edwards Brothers, Inc., Ann Arbor, Michigan, 1943).
18. Zintl and Schneider, Z. Elektrochem. 41, 771 (1935).
19. Grube and Wolf, Z. Elektrochem. 41, 675 (1935).
20. Pastorello, S., Gazz.chim. ital. 61, 47 (1931).
21. Komovsky and Maximow, Z. Krist. A92, 275 (1935).
22. Zintl and Woltersdorf, Z. Elektrochem. 41, 876 (1935).
23. Grube, Mohr, and Breuning, Z. Elektrochem. 41, 880 (1935).

24. Shamray and Saldau, Izvest. Akad. Nauk S.S.S.R. (khim.) 3, 631 (1937).

25. Grube and Schaufler, Z. Elektrochem. 40, 593 (1934).

26. Klemm and Struck, Z. anorg. Chem. 278, 117 (1955).

27. Baroni, A., Rend. reale accad. nazl. Lincei 16, 153 (1932).

28. Grube and Meyer, Z. Elektrochem. 40 771 (1934).

29. Nowotny, H., Z. Metallkunde 33, 388 (1941).

30. Grube and Klaiber, Z. Elektrochem. 40, 745 (1934).

31. Rollier and Arreghini, Z. Krist. 101, 470 (1939).

32. Zintl and Brauer, Z. Elektrochem. 41, 102 (1935).

33. Brill, R., Z. Krist. 65, 94 (1927).

34. Brauer and Zintl, Z. physik. Chem. B37, 323 (1937).

35. Grube, Vosskühler, and Schlecht, Z. Elektrochem. 40, 270 (1934).

36. Zintl and Brauer, Z. Elektrochem. 41, 297 (1935).

37. Zintl, Harder, and Dauth, Z. Elektrochem. 40, 588 (1934).

38. Laves and Wallbaum, Z. anorg. Chem. 250, 110-120 (1942).

39. Böhm and Klemm, Z. anorg. Chem. 243, 69-85 (1939).

40. Perlitz and Aruja, Z. Krist. A100, 157-166 (1938).

41. Haucke, W., Z. Elektrochem. 43, 712-719 (1937).

42. Pauling, L., J. Am. Chem. Soc. 45, 2777-2780 (1923).

43. Zintl and Neumayr, Z. physik. Chem. 20, 272-275 (1933).

44. Zintl and Dullenkopf, Z. physik. Chem. B16, 193 (1932).

45. Zintl and Harder, Z. physik. Chem. B34, 238-254 (1936).

46. Hansen, M., op. cit., p. 792.

47. Hansen, M., op. cit., p. 933.

48. Hansen, M., op. cit., p. 838.

49. Zintl and v. Baumbach, Z. anorg. Chem. 198, 88-101 (1931).

50. Goria, C., Gazz. chim. ital. 65 (2), 1226-1230 (1935).

51. Sommer, A., Nature 152, 215 (1943).

52. Hansen, M., op, cit., p. 778.

53. Allaria, S., Atti reale accad. sci. Torino, Classe sci. fis. mat. e nat. 78, 145 (1942-3).

54. Grube and Schmidt, Z. Elektrochem. 42, 201-209 (1936).

55. Hohmann, E., Z. anorg. Chem. 257, 113-126 (1948).

56. Grube and Botzenhardt, Z. Elektrochem. 48, 418 (1942).

57. Hansen, M., op. cit., p. 931.

58. Hansen, M., op. cit., p. 841.

59. Ethyl Corporation circular (1953).

60. Nowotny and Scheil, Metallforschung 2, 76-80 (1947).

61. Shoemaker, Marsh, Ewing, and Pauling, Acta Cryst. 5, 637 (1952).

62. Nielsen and Baenziger, Acta Cryst. 7, 277 (1954).

63. Marsh and Shoemaker, Acta Cryst. 6, 199 (1953).

64. Inoue and Osugi, J. Electrochem. Soc. Japan 20, 502-504 (1952).

65. Klaiber, H., Z. Elektrochem. 42, 258-264 (1936).

66. Tin Research Institute (1949); reported by Smithells, C., "Metals Reference Book," p. 524 (Interscience Publishers Inc., New York, 1955).

67. Zintl, Goubeau, and Dullenkopf, Z. physik. Chem. A154, 4 (1931).

68. Peyronel, G., Gazz chim. ital. 82, 679 (1952).

69. Smith, D. P., Z. anorg. Chem. 56, 129 (1907).

70. Weibke and Biltz, Z. anorg. Chem. 232, 297 (1937).

71. Zintl and Haucke, Z. Elektrochem. 44, 104-111 (1938).

72. Zintl and Haucke, Naturwissenschaften 25, 717 (1937).

73. Degenkolbe and Sauerwald, Z. anorg. u. allgem. Chem. 270, 317 (1952).

74. Brauer, Georg, Stein, and Vollprecht, Z. Naturforsch. B2, 323 (1947).

75. Zintl and Harder, Z. physik. Chem. B16, 206 (1932).

76. Smith, D. P., Z. anorg. Chem. 56, 133 (1907).

77. Klemm, Sodomann, and Langmesser, Z. anorg. u. allgem. Chem. 241, 281 (1939).

78. Bravo, Griswold, and Kleinberg, J. Phys. Chem. 58, 18 (1954).

79. Parke, R., "Metals Handbook," p. 1209 (The American Society for Metals, Cleveland, Ohio, 1948).

80. Baenziger and Duwell, Acta Cryst. 7, 635 (1954).

81. Bent and Gilfallan, J. Am. Chem. Soc. 55, 3989 (1933).

82. Smith, D. P., Z. anorg. Chem. 56, 112,113 (1907).

83. Tammann and Rüdiger, Z. anorg. Chem. 192, 26 (1930).

84. Smith, D. P., Z. anorg. Chem. 56, 125 (1907).

85. Ehrhorn, Weibke, Blitz, Z. anorg. Chem. 232, 307 (1937).

86. Klemm and Hauschulz, Z. Elektrochem. 45 (5), 346-354 (1939).

87. Baenziger, Nielsen, and Dowell, U. S. Atomic Energy Comm. Report No. AECU - 2279 (1952).

88. Schleede and Wellmann, Z. physik. Chem. B18, 1-28 (1932).

89. Anderson, Greenblatt, and Sommer, U. S. Atomic Energy Comm. Report No. AECU - 2949 (1954).

90. Biltz, Weibke, and Eggers, Z. anorg. Chem. 219, 119-128 (1934).

91. Berry and Raynor, Nature 171, 1078-1079 (1953).

92. Herbstein and Averbach, U. S. Atomic Energy Comm. Report No. NYO - 7046 (1954).

93. Baenziger, Nielsen, and Duwell, U. S. Atomic Energy Comm. Report No. COO - 127 (1953-54).

94. Stillwell and Robinson, J. Am. Chem. Soc. 55, 127-129 (1933).

PART III: STRUCTURE DETAILS

A 1: O_h^5--Fm3m

A=4: atoms at $000;\frac{1}{2}0\frac{1}{2};\ \frac{11}{22}0;0\frac{11}{22}$

Reported compounds: Li_3Cd

Remarks: Implied in this structure is a random distribution of the atomic species on the lattice sites. This probably is not true at low temperatures.

A 3: D_{6h}^4--$P6_3/mmc$

A=2: atoms at 1/3,2/3,1/4; 2/3,1/3,3/4

Reported compounds: $LiCd_3$ and $LiZn_9$

Remarks: See Remarks under A 1 structure.

B 2: O_h^1--Pm3m

A=2: ordered β-brass or CsCl structure
with Cs (O_h): 000
Cl (O_h): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Reported compounds: LiAg, LiCd, LiHg, LiTl, and LiPb

Remarks: LiAl was originally reported in this structure, but more recent work indicates the B 32 structure. LiCd has also been reported in both B 2 and B 32 structures, but which is the correct structure for LiCd is less clear.

B 32: O_h^7--Fd3m

A=16: NaTl structure
with 8 Na (T_d): $000;\frac{1}{4}\frac{1}{4}\frac{1}{4}$; +F. C.
8 Tl (T_d): $\frac{1}{2}\frac{1}{2}\frac{1}{2};\frac{3}{4}\frac{3}{4}\frac{3}{4}$; +F. C.
[F. C. = add $000;\frac{1}{2}0\frac{1}{2};\frac{11}{22}0;0\frac{11}{22}$; and $0\frac{11}{22}$ to all coordinates]

Reported compounds: LiZn, LiCd, LiAl, LiGa, LiIn, NaTl, and NaIn

Remarks: See Remarks under B 2.

C 1: O_h^5--Fm3m

A=12: fluorite structure, CaF_2
with 4 Ca (O_h): 000 +F. C.
8 F (T_d): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ +F. C.

Reported compounds: Li_2S, Li_2Se, Li_2Te, Na_2O, Na_2S, Na_2Se, Na_2Te, K_2Se, and K_2Te.

C 14: D_{6h}^4--$P6_3/mmc$

A=12: Laves Phase--$MgZn_2$ structure
with 4 Mg (C_{3v}): $\pm(1/3,2/3,z;\ 1/3,2/3,1/2-z)$; $z\approx 1/16$
2 Zn (D_{3d}): $000;00\frac{1}{2}$
6 Zn (C_{2v}): $\pm(x,2x,\frac{1}{4};\ \bar{2}x,\bar{x},\frac{1}{4};\ x,\bar{x},\frac{1}{4})$; $x\approx -1/6$

Reported compounds: Li_2Ca, Na_2K.

C 15: O_h^7--Fd3m

A=24: Laves Phase--$MgCu_2$ structure
with 8 Mg (T_d): $000;\frac{1}{4}\frac{1}{4}\frac{1}{4}$ +F. C.
16 Cu (D_{3d}): 5/8,5/8,5/8; 7/8,7/8,5/8; 7/8,5/8,7/8; 5/8,7/8,7/8 +F. C.

Reported compounds: KBi_2, $NaAu_2$.

C 16: D_{4h}^{18}--I4/mcm

A=12: $CuAl_2$ structure
with 4 Cu (D_4): $\pm(00\frac{1}{4})$ B. C.
8 Al (C_{2v}): $\pm(x,\frac{1}{2}+x,0;\ \frac{1}{2}+x,\bar{x},0)$ +B. C.
/B. C. = add 000 and $\frac{1}{3}\frac{1}{2}\frac{1}{2}$ to all coordinates/

Reported compounds: Na_2Au with x=0.160.

C 32: D_{6h}^1--P6/mmm

A=3: AlB_2 structure
with 1 Al (D_{6h}): 000
2 B (D_{3h}): 1/3,2/3,1/2; 2/3,1/3,1/2

Reported compounds: $NaHg_2$.

D O_3: O_h^5--Fm3m

A=16: $BiLi_3$ structure
with 4 Bi (O_h): 000 +F. C.
4 Li (O_h): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ +F. C.
8 Li (T_d): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ +F. C.

Reported compounds: Li_3Hg, Li_3Sb, Li_3Bi

Remarks: Li_3Sb exists also in the hexagonal D O_{18} structure.

D O_{18}: D_{6h}^4--$P6_3/mmc$

A=8: Na_3As structure
with 2 As (D_{3h}): $\pm(1/3,2/3,1/4)$
2 Na (D_{3h}): $\pm(00\frac{1}{4})$
4 Na (C_{3v}): $\pm(1/3,2/3,z;\ 2/3,1/3,1/2+z)$; z=0.583

Reported compounds: Li_3Pb, Li_3Sb, Li_3P, Li_3As, Na_3As, Na_3P, Na_3Sb, Na_3Bi, K_3As, K_3Sb, K_3Bi, Rb_3Sb

Remarks: See also D O_3.

D O_{19}: D_{6h}^4--$P6_3/mmc$

A=8: Mg_3Cd structure
with 2 Cd (D_{3h}): $\pm(1/3,2/3,1/4)$
6 Mg (C_{2v}): $\pm(2x,x,\frac{1}{4};\ \bar{x},x,\frac{1}{4};\ \bar{x},2x,\frac{1}{4})$; $x\approx 1/6$

Reported compounds: $LiHg_3$.

D 2_3: O_h^6--Fm3c

A=112: $NaZn_{13}$ structure
with 8 Na (O): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ +F. C.
8 Zn (T_h): $000;\frac{1}{2}\frac{1}{2}\frac{1}{2}$ +F. C.
96 Zn (C_s): $\pm(0,y,z;\ \mathcal{P};\ \frac{1}{2},z,y;\ \mathcal{P};\ 0,y,\bar{z};\ \mathcal{P};\ \frac{1}{2},\bar{z},y;\ \mathcal{P})$ +F. C.
[$\mathcal{P}$ = permutations]

Reported compounds: $NaZn_{13}$ with y=0.1806 and z=0.1192,
$RbCd_{13}$ with y=0.178 and z=0.122,
KZn_{13}--y and z not precisely determined,
KCd_{13}--y and z not precisely determined.

D 8_{1-3}: O_h^9--Im3m; T_d^3--I$\bar{4}$3m; and T_d^1--P$\bar{4}$3m

A=52: γ-brass structures. The basic structure consists of a cubic unit cell whose edge is three times the edge of a simple body-centered cubic cell. From this large cell of 54 atomic sites is abstracted 2 atomic sites with small attendant shifts in parameters of some of the 52 occupied sites. The space group depends upon the formula of the compound and the atomic species occupying the various atomic sites.

Reported compounds: Li_3Ag (reported formula varies from $Li_{12}Ag$ to Li_3Ag), $Li_{10}Pb_3$ (Li_5Pb_2)

Remarks: γ-brass structures usually exhibit extensive composition variation.

D 8_6: T_d^6--I$\bar{4}$3d

A=76: $Cu_{15}Si_4$ type
with 12 Cu (S_4): 0,1/4,3/8; $\mathcal{R}$; 0,3/4,1/8; $\mathcal{R}$ +B. C.
48 Cu (C_1): x,y,z; $\mathcal{R}$; x,$\bar{y}$,$\frac{1}{2}$-z; $\mathcal{R}$; $\frac{1}{2}$-x,y,$\bar{z}$; $\mathcal{R}$; $\bar{x}$,$\frac{1}{2}$-y,z; $\mathcal{R}$; $\frac{1}{4}$+y,$\frac{1}{4}$+x,$\frac{1}{4}$+z; $\mathcal{R}$; $\frac{1}{4}$-y,$\frac{1}{4}$+x,3/4-z; $\mathcal{R}$; $\frac{1}{4}$+y,3/4-x,$\frac{1}{4}$-z; $\mathcal{R}$; 3/4-y,$\frac{1}{4}$-x,$\frac{1}{4}$+z; $\mathcal{R}$; +B. C: x=0.12, y=0.16, z=0.04
16 Si (C_3): xxx;x,$\bar{x}$,$\frac{1}{2}$-x; $\mathcal{R}$; $\frac{1}{4}$+x,$\frac{1}{4}$+x,$\frac{1}{4}$+x; $\frac{1}{4}$-x, $\frac{1}{4}$+x,3/4-x; $\mathcal{R}$: x=0.208

Reported compounds: $Na_{15}Sn_4$, $Na_{15}Pb_4$ ($Na_{31}Pb_8$).

L 10: D_{4h}^1--P4/mmm

A=2: CuAu type superlattice
with 1 Cu (D_{4h}): 000
1 Au (D_{4h}): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Reported compounds: LiBi, NaBi, NaSb (?).

L 12: O_h^1--Pm3m

A=4: Cu_3Au type superlattice
with 1 Au (O_h): 000
3 Cu (D_{4h}): $\frac{1}{2}0\frac{1}{2}$; $0\frac{1}{2}\frac{1}{2}$; $\frac{1}{2}\frac{1}{2}0$

Reported compounds: Na_2Pb_5

Remarks: The formula makes mandatory some statistical occupancy of sites. In all probability the assignment of this compound to this structure is erroneous. See NaPb.

--- D_{4h}^{20}--I4/acd

A=64: NaPb structure
with 32 Pb (C_1): $\underline{x},\underline{y},z$; $\underline{x},\bar{y},\frac{1}{2}+z$; $\underline{x},\frac{1}{2}+y,\frac{1}{4}-z$; $\underline{x},\frac{1}{2}-y,3/4-z$; $\underline{x},y,\underline{z}$; $x,y,\frac{1}{2}+z$; $\underline{x},\frac{1}{2}-y,\frac{1}{4}-z$; $x,\frac{1}{2}+y,3/4-z$; $\underline{y},\underline{x},\underline{z}$; $\underline{y},\underline{x},\frac{1}{2}-z$; $y,\frac{1}{2}+x,\frac{1}{4}+z$; $\underline{y},\frac{1}{2}+x,3/4+z$; y,x,z; $y,x,\frac{1}{2}-z$; $y,\frac{1}{2}-x,\frac{1}{4}+z$; $y,\frac{1}{2}-x,3/4+z$; +B. C: $x=0.0696 \pm 0.0013$, $y=0.1186 \pm 0.0012$, $z=0.9383 \pm 0.0008$

16 Na (C_2): $\underline{1/4},x,1/8$; $3/4,\bar{x},\underline{1/8}$; $3/4,x,5/8$; $1/4,\underline{x},5/8$; $x,1/4,3/8$; $x,3/4,3/8$; $x,3/4,7/8$; $x,1/4,\underline{7/8}$; +B. C: $x \approx \underline{1/8}$

16 Na (C_2): $x,x,\frac{1}{4}$; $x,\underline{x},\frac{1}{4}$; $x,x,3/4$; $x,x,\underline{3/4}$; $x,\frac{1}{2}+x,0$; $x,\frac{1}{2}-x,0$; $x,\frac{1}{2}-x,\frac{1}{2}$; $x,\frac{1}{2}+x,\frac{1}{2}$; +B. C: $x \approx 1/8$

Remarks: $R_{(\text{powder data})} = \dfrac{\Sigma|F_o - F_c|}{\Sigma|F_o|} = 14.5\%$; least squares refinement of Pb positions; F_o-F_c refinement of Na positions.

--- D_{4h}^{14}--$P4_2/mnm$

A=20: Na_3Hg_2 structure
with 8 Hg (C_s): $(x,x,z$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2}+z$; $\bar{x},\bar{x},z$; $\frac{1}{2}-x,\frac{1}{2}+x,\frac{1}{2}+z)$: $x=0.125 \pm 0.0005$, $z=0.190 \pm 0.001$

4 Na (C_{2v}): $\pm(x,\bar{x},0$; $\frac{1}{2}+x,\frac{1}{2}+x,\frac{1}{2})$: $x=0.210 \pm 0.010$

4 Na (C_{2v}): $\pm(x,x,0$; $\frac{1}{2}+x,\frac{1}{2}-x,\frac{1}{2})$: $x=0.368 \pm 0.010$

4 Na (C_{2h}): $0\frac{1}{2}0;\frac{1}{2}00;0\frac{1}{2}\frac{1}{2};\frac{1}{2}0\frac{1}{2}$

Remarks: $R_{(hko)} = \dfrac{\Sigma|F_o - F_c|}{\Sigma|F_o|} = 8.4\%$

--- D_{2h}^{17}--Cmcm

A=16: NaHg structure
with 8 Hg (C_s): $\pm(x,y,\frac{1}{4}$; $\bar{x},y,\frac{1}{4}$; $\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{4}$; $\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{4})$: $x=0.212 \pm 0.0015$, $y=0.088 \pm 0.0010$

4 Na (C_{2v}): $\pm(0,y,\frac{1}{4}$; $\frac{1}{2},\frac{1}{2}+y,\frac{1}{4})$: $y=0.368 \pm 0.010$

4 Na (C_{2v}): $\pm(0,y,\frac{1}{4}$; $\frac{1}{2},\frac{1}{2}+y,\frac{1}{4})$: $y=0.814 \pm 0.006$

Remarks: $R = \dfrac{\Sigma|F_o - F_c|}{\Sigma|F_o|} = 20.3\%$

--- O_h^1--Pm3m

A=36: KHg_{11} structure
with 3 K (D_{4h}): $\frac{1}{2}00;0\frac{1}{2}0;00\frac{1}{2}$
1 Hg (O_h): 000
8 Hg (C_{3v}): $\pm(xxx;x\bar{x}\bar{x};\bar{x}x\bar{x};\bar{x}\bar{x}x)$: $x\cong0.155$
12 Hg (C_{2v}): $\pm(xx0;x0x;0xx;x\bar{x}0;0x\bar{x};\bar{x}0x)$: $x\cong0.345$
12 Hg (C_{2v}): $\pm(xx\frac{1}{2};\frac{1}{2}xx;x\frac{1}{2}x;x\bar{x}\frac{1}{2};\frac{1}{2}x\bar{x};\bar{x}\frac{1}{2}x)$: $x\cong0.275$

--- D_{6h}^4--$P6_3/mmc$

A≈3: Li_7Zn_{18} structure
with 2 Zn (D_{3h}): $\pm(1/3,2/3,1/2)$
~0.8 Li (D_{3d}): $000;00\frac{1}{2}$

Reported compounds: Li_7Zn_{18} (and formula variations)

Remarks: Evidently a high percentage of the Li sites are unoccupied, and the symmetry would indicate that the vacancies are random.

--- C_i^1--$P\bar{1}$

A=8: KHg structure
with 2 Hg (C_1): $\pm(xyz)$: x=0.198, y=0.101, z=0.286
2 Hg (C_1): $\pm(xyz)$: x=0.877, y=0.313, z=0.049
2 K (C_1): $\pm(xyz)$: x=0.281, y=0.653, z=0.489
2 K (C_1): $\pm(xyz)$: x=0.675, y=0.794, z=0.166

Remarks: Least squares refinement of parameters.